

Thermodynamic Functions of Some Moieties Involving Heterocyclic Analogues of Cyclopentadiene

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ABSTRACT

New metal complexes of bivalent copper, cobalt, nickel and palladium metal ions with [p-((p-aminophenyl)thio)-phenylpyrrole-2-yl-ethylidene] have been synthesized. The co-ordinating centres and their geometries have been confirmed from spectroscopic-IR, electronic, UV, Raman, NMR studies.

Some thermodynamic functions viz., Enthalpy (ΔH), heat capacity (C_p), free energy $-\left(\frac{F-E}{T}\right)$ and

entropy (ΔS) of the molecules have been calculated using rigid rotor harmonic oscillator approximation. The data used by the program are molecular frequencies, moments of inertia and symmetry parameters. These calculations are carried out at different temperatures from 100 K to 1500 K.

Key Words : Palladium metal, rigid motor harmonic oscillator, pyrsole ring